

# On the Number of Many-to-Many Alignments of Multiple Sequences

STEFFEN EGER

*Computer Science Department, Goethe University Frankfurt am Main  
Robert-Mayer-Straße 10, Frankfurt, Germany  
e-mail: steeger@em.uni-frankfurt.de*

## ABSTRACT

We count the number of alignments of  $N \geq 1$  sequences when match-up types are from a specified set  $S \subseteq \mathbb{N}^N$ . Equivalently, we count the number of non-negative integer matrices whose rows sum to a given fixed vector and each of whose columns lie in  $S$ . We provide a new asymptotic formula for the case  $S = \{(s_1, \dots, s_N) \mid 1 \leq s_i \leq 2\}$ .

*Keywords:* Alignment, composition, sum of discrete random variable, lattice path

## 1. Introduction

Alignments of sequences arise in computational biology and in computational linguistics. In computational biology, aligning DNA sequences is a standard task. In computational linguistics, aligning (historical) variants of linguistic forms is a field of study (see [8]). In addition, alignments of sequences arise in computational linguistics either in (machine) translation, where words from different languages are matched up, or in related string-to-string translation tasks such as letter-to-sound conversion, where the task is to translate a letter string into a phonetic representation, or in lemmatization, where the task is to translate a word form into a canonical lexicon representation.

Traditionally, an alignment of  $N$  (for an integer  $N \geq 2$ ) sequences of various lengths is defined as a manner of inserting blanks into the  $N$  sequences such that all have equal length. For example, given  $\mathbf{x} = x_1$ ,  $\mathbf{y} = y_1y_2$  and  $\mathbf{z} = z_1z_2z_3$ , three (out of 239 possible) alignments of  $\mathbf{x}, \mathbf{y}$  and  $\mathbf{z}$  are:

$$\begin{array}{ccccccc}
 x_1 & - & - & & x_1 & - & - & - & & - & - & x_1 \\
 y_1 & y_2 & - & & y_1 & - & y_2 & - & & y_1 & y_2 & - \\
 z_1 & z_2 & z_3 & & z_1 & z_2 & - & z_3 & & z_1 & z_2 & z_3
 \end{array} \quad (\clubsuit)$$

As can be seen, each such alignment has the property that, in each position, an element of one of the sequences is matched up with one or zero elements from each of the other sequences. In computational linguistics, alignments in which *subsequences of length  $\geq 1$*  from the different sequences are matched up with each other (**‘many-to-many matches’**) are oftentimes more plausible and also more frequently made of use of (see [15, 19]). When we allow, for example, in addition to the above specification, matches-up of length up to 2, there are several further alignments of  $\mathbf{x}, \mathbf{y}$  and  $\mathbf{z}$ , including:

$$\begin{array}{ccccccc}
 x_1 & - & & - & x_1 & - & - & x_1 \\
 y_1 y_2 & - & & y_1 y_2 & - & - & y_1 y_2 & - \\
 z_1 z_2 & z_3 & & z_1 z_2 & z_3 & & z_1 & z_2 & z_3
 \end{array}
 \quad (\clubsuit\clubsuit)$$

Several works have counted the number of alignments of two and more (**‘multiple’**) sequences, see [1, 9, 11, 13, 17, 29, 32, 34]. These works typically referred to the traditional definition of multiple alignments outlined above. In this note, we count the number of alignments of  $N$  sequences in which match-up types lie in an arbitrary set  $S$ . The set  $S$  may (but need not) contain many-to-many matches in the above sense. Hence, our approach generalizes the traditional setup.

This work is structured as follows. Section 2 gives a precise definition of multiple alignments as we consider here. Section 3 places our work in context. Section 4 outlines three theorems on multiple many-to-many alignments, which we will make use of in Section 5: (i) a recursion, which easily allows to calculate the number of alignments for arbitrary  $S$ ; (ii) the multivariate generating function for the number of multiple many-to-many alignments, from which we can derive asymptotics; and (iii) a summation of the number of alignments in terms of binomial coefficients, which allows for specifying closed-form formulas. Finally, Section 5 surveys and outlines formulas for specific  $S$ . In particular, we derive a new asymptotic for the number of multiple many-to-many alignments in which subsequences of length 1 or 2 are matched up with each other.

## 2. Defining multiple many-to-many alignments

For  $N \geq 1$  fixed, let  $\mathbf{x}_1, \dots, \mathbf{x}_N$  be  $N$  sequences (over arbitrary alphabets) of finite lengths  $\ell_1, \dots, \ell_N$ , respectively. We define a multiple many-to-many alignment of the  $N$  sequences with respect to a set  $S$  of ‘allowable steps’. The set  $S$  defines the valid match-up operations.

**Definition 1** Let  $S$  be an arbitrary subset of  $\mathbb{N}^N$ , where  $\mathbb{N}$  is the set of non-negative integers. We define an  $S$ -alignment of  $\mathbf{x}_1, \dots, \mathbf{x}_N$  as any  $N \times k$  matrix  $\mathbf{A}$ , for some  $k \geq 1$ , with non-negative integer entries such that

- Each row of  $\mathbf{A}$  sums to the length of the respective sequence:  $\mathbf{A}\mathbb{1}_k = \begin{pmatrix} \ell_1 \\ \vdots \\ \ell_N \end{pmatrix}$ . Here,  $\mathbb{1}_k$  is the vector, of size  $k$ , with all entries equal to 1.
- Each column of  $\mathbf{A}$  is an element of  $S$ .<sup>1</sup>

**Example 1** When  $S = \{(1, 1), (1, 2), (2, 1)\}$ , there are seven  $S$ -alignments of a string of length 4 and a string of length 5. These are:

$$\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 2 \end{pmatrix} \quad \begin{pmatrix} 1 & 2 & 1 \\ 2 & 1 & 2 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & 2 \\ 2 & 2 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 1 \end{pmatrix}$$

**Example 2** The traditional definition of multiple alignment of  $N$  sequences is retrieved when  $S = \{(s_1, \dots, s_N) \mid 0 \leq s_i \leq 1\} - \{(0, \dots, 0)\}$ . Thus, for  $N = 2$ ,  $S$  has the form  $\{(1, 0), (0, 1), (1, 1)\}$  and for  $N = 3$ ,  $S$  has the form

$$\{(0, 0, 1), (0, 1, 0), (1, 0, 0), (0, 1, 1), (1, 0, 1), (1, 1, 0), (1, 1, 1)\}.$$

The three  $S$ -alignments in () have the matrix representations

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$

respectively.

**Example 3** The three alignments given in () have the matrix representations

$$\begin{pmatrix} 1 & 0 \\ 2 & 0 \\ 2 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 2 & 0 \\ 2 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$

respectively. Hence, they are  $S$ -alignments of  $\mathbf{x}, \mathbf{y}, \mathbf{z}$  for any  $S \supseteq \{(1, 2, 2), (0, 0, 1), (0, 2, 2), (1, 0, 1), (0, 2, 1)\}$ .

<sup>1</sup>In our notation below, we do not distinguish column from row vectors.

For the remainder, we use the following **notation**. We denote a tuple  $(s_1, \dots, s_N)$  also by  $\mathbf{s}$  when this causes no confusion. We write  $\mathbf{A}_i$  for column  $i$  of matrix  $\mathbf{A}$ . We denote by  $a_S(\ell_1, \dots, \ell_N)$  the number of  $S$ -alignments of sequences of lengths  $\ell_1, \dots, \ell_N$ . We denote by  $a_S(\ell_1, \dots, \ell_N; k)$  the number of  $S$ -alignments of sequences of lengths  $\ell_1, \dots, \ell_N$  when the number of columns ( $=$  *length*, or number of *parts*, of the alignment) of the respective matrices is exactly  $k$ . We let  $A_S(\ell_1, \dots, \ell_N)$  and  $A_S(\ell_1, \dots, \ell_N; k)$ , respectively, denote the corresponding sets of  $S$ -alignments. We write  $\mathbf{0}_N$  for the vector  $(0, \dots, 0) \in \mathbb{N}^N$ .

### 3. Background

Multiple many-to-many alignments as we consider here generalize the concept of *vector compositions* introduced in [2]. In fact, vector compositions are  $S$ -alignments in which  $S = \mathbb{N}^N - \{\mathbf{0}_N\}$ . For the same  $S$ , Munarini et al. [25] introduce *matrix compositions*. These are matrices whose entries sum to a positive integer  $n$  and whose columns are non-zero. We find that the number  $c^{(N)}(n)$  of matrix compositions with  $N$  rows satisfies  $c^{(N)}(n) = \sum_{\ell_1 + \dots + \ell_N = n} a_S(\ell_1, \dots, \ell_N)$ .

Multiple many-to-many alignments are also closely related to *lattice path combinatorics* (see [33]). Lattice paths are paths from the origin  $\mathbf{0}_N$  to some point  $(\ell_1, \dots, \ell_N)$  in which each step lies in some set  $S$ . In our case, each coordinate of each step  $\mathbf{s} \in S$  is non-negative.

When  $S$  is fixed and finite, then the class

$$L_S = \{\mathbf{A} \in \mathbb{N}^{N \times k} \mid \mathbf{A} \text{ satisfies Definition 1 for some } (\ell_1, \dots, \ell_N) \text{ and some } k\}$$

is clearly a *regular language*. In fact,  $L_S$  is given by the regular expression  $(\mathbf{s}_1 \mid \dots \mid \mathbf{s}_r)^+$ , where  $\mathbf{s}_1, \dots, \mathbf{s}_r$  are the elements of  $S$ . Munarini et al. [25] specify an encoding showing that  $L_S$  is regular even when  $S = \mathbb{N}^N - \{\mathbf{0}_N\}$ .

Multiple many-to-many alignments are also related to *sums of discrete multivariate random variables*. In fact, let  $X_1, \dots, X_k$  be independently and identically distributed random vectors, each of whose range is  $S$ . Then,

$$P[X_1 + \dots + X_k = (\ell_1, \dots, \ell_N)] = \sum_{\mathbf{A} \in A_S(\ell_1, \dots, \ell_N; k)} P[\mathbf{A}_1] \cdots P[\mathbf{A}_k].$$

When each  $X_i$  is uniformly distributed on  $S$ , then

$$P[X_1 + \dots + X_k = (\ell_1, \dots, \ell_N)] = \frac{1}{|S|^k} a_S(\ell_1, \dots, \ell_N; k).$$

Since the sum  $X_1 + \dots + X_k$  is asymptotically normal, the last equality allows to approximate  $a_S(\ell_1, \dots, \ell_N; k)$  by a normal curve in the spirit of [14].

Finally, it is well-known that alignment problems are closely related to the edit distance problem [23]. Edit distance measures the minimal number of insertions, deletions, and substitutions necessary to transform one string into another. Allowing steps in a set  $S$  would correspond to allowing transformation patterns as specified by  $S$ , such as insertion (via the step  $(0, 1)$ ), deletion  $((1, 0))$ , or more complex transformations such as inversion  $((2, 2))$ , expansion  $((1, 2))$  or squashing  $((2, 1))$  (see [13, 26]). Considering  $N \geq 2$  sequences further generalizes this setup.

#### 4. Counting the number of multiple many-to-many alignments

Theorem 1 outlines a recurrence which  $a_S(\ell_1, \dots, \ell_N)$  satisfies and which allows its efficient evaluation.

**Theorem 1** *The quantity  $a_S(\ell_1, \dots, \ell_N)$  satisfies the recurrence*

$$a_S(\ell_1, \dots, \ell_N) = \sum_{(s_1, \dots, s_N) \in S} a_S(\ell_1 - s_1, \dots, \ell_N - s_N)$$

with initial conditions  $a_S(0, \dots, 0) = 1$  and  $a_S(n_1, \dots, n_N) = 0$  whenever  $n_m < 0$  for some  $1 \leq m \leq N$ .

*Proof.* Each  $S$ -alignment of some length  $k$  is made up of a last column  $\mathbf{s} = (s_1, \dots, s_N) \in S$  and an arbitrary  $S$ -alignment of length  $k - 1$  of  $(\ell_1 - s_1, \dots, \ell_N - s_N)$ .  $\square$

Below we show sample Python<sup>2</sup> code that computes  $a_S(\ell_1, \dots, \ell_N)$  efficiently based on Theorem 1.

```

1  import itertools, numpy as np
2
3  def a(l, S):
4      # l = [l_1, ..., l_N]
5      N = len(l)
6      indices = [range(l_i+1) for l_i in l]
7      zero = tuple([0 for i in xrange(N)])
8      table = {}
9      for multiindex in itertools.product(*indices):
10         multiindex = tuple(multiindex)
```

<sup>2</sup>See [www.python.org](http://www.python.org).

```

11         if multiindex==zero:
12             table[multiindex]=1
13         else:
14             local = 0
15             for s in S:
16                 index = tuple(np.array(multiindex)-np.
17                               array(s))
18                 local += table.get(index,0)
19             table[multiindex] = local
20     return table[tuple(1)]

```

**Theorem 2** Let  $f(z_1, \dots, z_N) = \sum_{n_1, \dots, n_m \geq 0} a_S(n_1, \dots, n_m) z_1^{n_1} \cdots z_N^{n_m}$  be the multivariate generating function for the number of  $S$ -alignments. Then  $f(z_1, \dots, z_N)$  has the representation

$$f(z_1, \dots, z_N) = \frac{1}{1 - \sum_{(s_1, \dots, s_N) \in S} z_1^{s_1} \cdots z_N^{s_N}}.$$

*Proof.* The generating function for  $a_S(\ell_1, \dots, \ell_N; k)$  is easily seen to be

$$f(z_1, \dots, z_N; k) = \left( \sum_{s \in S} z_1^{s_1} \cdots z_N^{s_N} \right)^k.$$

The result then follows by summing over  $k$ .  $\square$

**Theorem 3** Let the elements in  $S$  be enumerated as  $\mathbf{s}_1, \mathbf{s}_2, \dots$ . Moreover, let  $k \geq 0$  and let

$$B_S(k, \ell_1, \dots, \ell_N) = \{(r_1, r_2, \dots, r_t) \mid r_i \geq 0, \sum_{i=1}^t r_i = k, \sum_{i=1}^t \mathbf{s}_i r_i = (\ell_1, \dots, \ell_N)\}.$$

Here,  $t$  is the size of  $S$ .<sup>3</sup> Then

$$a_S(\ell_1, \dots, \ell_N) = \sum_{k \geq 0} \sum_{(r_1, r_2, \dots, r_t) \in B_S(k, \ell_1, \dots, \ell_N)} \binom{k}{r_1, r_2, \dots, r_t}, \quad (1)$$

where  $\binom{k}{r_1, r_2, \dots, r_t} = \frac{k!}{r_1! r_2! \cdots r_t!}$  are the multinomial coefficients.

*Proof.* We first note that  $a_S(\ell_1, \dots, \ell_N) = \sum_{k \geq 0} a_S(\ell_1, \dots, \ell_N; k)$ . We then find the above formula for  $a_S(\ell_1, \dots, \ell_N; k)$  by matching up columns of the same type  $\mathbf{s}_i$ ;  $r_i$  is the *multiplicity* of column type  $\mathbf{s}_i$ .  $\square$

<sup>3</sup>When  $S$  has infinite size, then all  $r_i$  must be zero for which  $\mathbf{s}_i$  has a component that exceeds the corresponding component of  $(\ell_1, \dots, \ell_N)$ ; hence, only a finite and fixed number  $t'$  of indices in  $(r_1, r_2, \dots, r_t)$  can be non-zero in this case, too.

## 5. Special cases

### 5.1. The case $N = 1$

The case  $N = 1$ , which might be considered a degenerate case of an alignment, yields the number of  $S$ -restricted integer compositions (see [12, 18]) of  $\ell$ , i.e., the number of solutions  $(\pi_1, \dots, \pi_k)$  such that  $\pi_1 + \dots + \pi_k = \ell$ , and where each  $\pi_i \in S$ . Depending on  $S$ , there are several closed-form solutions for  $a_S(\ell)$  as exemplified in Table 1.

$S = \{1, 2, 3, \dots\}$	$a_S(\ell) = 2^{\ell-1}$
$S = \{1, 2\}$	$a_S(\ell) = F_{\ell+1}$
$S = \{2, 3, 4, \dots\}$	$a_S(\ell) = F_{\ell-1}$
$S = \{1, 3, 5, 7, \dots\}$	$a_S(\ell) = F_\ell$
$S = \{1, 2, \dots, M\}$	$a_S(\ell) \sim \frac{\phi^{\ell+1}}{G'(\sigma)}$

Table 1:  $a_S(\ell)$  for different  $S \subseteq \mathbb{N} - \{\mathbf{0}_1\}$ . Here,  $F_n$  denotes the  $n$ -th Fibonacci number (see, e.g., [16, 30]). Moreover,  $M \geq 1$  and  $\phi$  is the unique positive real solution to  $\frac{1}{X^1} + \dots + \frac{1}{X^M} = 1$ ,  $G(x) = x^1 + \dots + x^M$  and  $G'$  denotes the first derivative of  $G$ , and  $\sigma = 1/\phi$  (see [24]).

### 5.2. The case $N = 2$

#### 5.2.1. The case $S = \{(1, 0), (0, 1), (1, 1)\}$

The case  $S = \{(1, 0), (0, 1), (1, 1)\}$  is the classical case of alignments of exactly two sequences with (simple) matches and skips (see [1, 9]). It leads to the well-known *Delannoy numbers* (see [3]). The central Delannoy numbers are listed as integer sequence A001850 (see [31]). Table 2 provides two identities for  $a_S(\ell_1, \ell_2)$  and one approximate formula for the numbers. We note that the second formula immediately follows from Theorem 3 in a similar manner as for  $a_{\{(1,1),(1,2),(2,1)\}}(\ell_1, \ell_2)$  in Section 5.2.2.

#### 5.2.2. The case $S = \{(1, 1), (1, 2), (2, 1)\}$

The case  $S = \{(1, 1), (1, 2), (2, 1)\}$  is given as integer sequence A191588. Its diagonal  $a_S(\ell, \ell)$  is given as sequence A098479. Table 3 lists two formulas, whose proofs we sketch below. A more general formula for the case  $\{(1, 1), (1, 2), \dots, (1, A)\} \cup \{(2, 1), \dots, (B, 1)\}$ , for  $A, B \geq 2$ , is provided in [13].

Exact	$\sum_{d \geq 0} 2^d \binom{\ell_1}{d} \binom{\ell_2}{d}$
	$\sum_{d \geq 0} \frac{(\ell_1 + \ell_2 - d)!}{d! (\ell_1 - d)! (\ell_2 - d)!}$
Approximate	$\left(\frac{r + \ell_2}{\ell_1}\right)^{\ell_1} \left(\frac{r + \ell_1}{\ell_2}\right)^{\ell_2}$

Table 2: Exact formulas and approximations for Delannoy numbers. Here  $r = \sqrt{\ell_1^2 + \ell_2^2}$  (see [21, 22]).

$$\begin{array}{ll}
 (\star) & \sum_{k=0}^{\ell_1} \binom{k}{2k-\ell_1} \binom{2k-\ell_1}{\ell_2-k} \\
 (\star\star) & \sum_{k=\lceil \frac{\max\{\ell_1, \ell_2\}}{2} \rceil}^{\min\{\ell_1, \ell_2\}} \sum_{j \geq 0} (-1)^j \binom{k}{j} \binom{k-j}{\ell_1-k-j} \binom{k-j}{\ell_2-k-j}
 \end{array}$$

Table 3: Closed-form formulas for  $a_{\{(1,1), (1,2), (2,1)\}}(\ell_1, \ell_2)$ .

*Proof.* Proof of formula  $(\star)$ : Let  $S = \{(1,1), (1,2), (2,1)\}$ . The constraints on the multiplicities  $(r_1, r_2, r_3)$  in Eq. (1), Theorem 3, can then be rewritten as

$$\begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 1 \end{pmatrix}^{-1} \begin{pmatrix} k \\ \ell_1 \\ \ell_2 \end{pmatrix} = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 0 & 1 \\ -1 & 1 & 0 \end{pmatrix} \begin{pmatrix} k \\ \ell_1 \\ \ell_2 \end{pmatrix}$$

which leads to the formula  $\sum_{k \geq 0} \frac{k!}{(\ell_1 - k)! (\ell_2 - k)! (3k - \ell_1 - \ell_2)!}$ , which is equivalent to the formula indicated.  $\square$

*Proof.* Proof of formula  $(\star\star)$ : This identity follows by applying the inclusion/exclusion principle to the sets  $A_i =$  set of  $2 \times k$  matrices with entries in  $\{1, 2\}$  whose first and second row sum to  $\ell_1$  and  $\ell_2$ , respectively, such that column  $i$  consists of 2's. For fixed number  $k$  of columns, we note that  $a_S(\ell_1, \ell_2; k) = |A_1^c \cap \dots \cap A_k^c|$ .  $\square$

### 5.2.3. The case $S = \{(1,1), (1,2), (2,1), (2,2)\}$

The diagonals  $a_S(\ell, \ell)$  of this case are listed as integer sequence A051286. They are also known as *Whitney numbers* of the fence poset  $A_\ell$ , see [7]. Table 4 below lists an exact formula for  $a_S(\ell_1, \ell_2)$ , which can be derived as sketched in Section 5.4, and an approximate formula for  $a_S(\ell, \ell)$  which is provided in the comments for the respective integer sequence.



Exact	$\sum_{k \geq 0} \binom{\ell_1 - k}{k} \binom{\ell_2 - k}{k}$
Approximate	$\sqrt{3 + \frac{7}{\sqrt{5}}} \cdot \frac{(\frac{1+\sqrt{5}}{2})^{2\ell}}{\sqrt{8\pi\ell}}$

Table 4: Exact and approximate formulas for  $a_{\{(1,1),(1,2),(2,1),(2,2)\}}(\ell_1, \ell_2)$  and  $a_{\{(1,1),(1,2),(2,1),(2,2)\}}(\ell, \ell)$ , respectively.

#### 5.2.4. The case $S = \{(x, y) \mid x \geq 1, y \geq 0\}$

The diagonal  $a_S(\ell, \ell)$  of this case is integer sequence A047781. A closed-form formula for  $a_S(\ell_1, \ell_2)$  can easily be established as (see [20])

$$\sum_{k \geq 0} \binom{\ell_1 - 1}{k - 1} \binom{\ell_2 + k - 1}{k - 1}.$$

This result follows from Section 5.4 and by noting that the number of *compositions* (that is,  $\{1, 2, 3, \dots\}$ -restricted integer compositions in the sense of Section 5.1) of  $n$  with exactly  $k$  parts is  $c_{\{1,2,3,\dots\}}(n, k) = \binom{n-1}{k-1}$  and the number of *weak compositions* ( $\mathbb{N}$ -restricted integer compositions in the above sense) of  $n$  with exactly  $k$  parts is  $c_{\{0,1,2,3,\dots\}}(n, k) = \binom{n+k-1}{k-1}$ . A comment for the integer sequence lists the asymptotic

$$a_S(\ell, \ell) \sim \frac{2^{1/4} \cdot (3 + 2\sqrt{2})^\ell}{4\sqrt{\pi\ell}}.$$

#### 5.2.5. Similar cases

We may construct more such examples *ad libitum*. For instance, the case  $S = \{(1, 1), (1, 3), (3, 1)\}$  is listed as integer sequence A098482. The case  $S = \{(1, 0), (1, 1), (1, 2), (2, 1)\}$  is listed as integer sequence A191354. When  $S = \{(x, y) \mid 1 \leq x \leq 3, 1 \leq y \leq 3\}$ , then similarly as for the Whitney numbers, we may derive

$$a_S(\ell_1, \ell_2) = \sum_{k \geq 0} \left( \sum_{i \geq 0} \binom{k}{i} \binom{k-i}{\ell_1 - k - 2i} \right) \left( \sum_{i \geq 0} \binom{k}{i} \binom{k-i}{\ell_2 - k - 2i} \right).$$

#### 5.3. The case $N = 3$

Let  $S = \{(x, y, z) \mid 0 \leq x, y, z \leq 1\} - \{\mathbf{0}_3\}$ . Then,  $a_S(\ell, \ell, \ell)$  is integer sequence A126086. The comments for this sequence list as approximate formula:

$$a_S(\ell, \dots, \ell) \sim c \cdot d^\ell,$$

where  $d = 12 \cdot 2^{2/3} + 15 \cdot 2^{1/3} + 19$  and  $c$  is a specified constant. Further formulas can be retrieved as special cases of the results in Section 5.5.

5.4. *The case  $S = S_{X_1} \times \cdots \times S_{X_N}$*

If  $S_{X_1}, \dots, S_{X_N} \subseteq \mathbb{N}$  are base sets and  $S = S_{X_1} \times \cdots \times S_{X_N}$  ('independence'), then  $a_S(\ell_1, \dots, \ell_N)$  is given by

$$\sum_{k \geq 0} c_{S_{X_1}}(\ell_1; k) \cdots c_{S_{X_N}}(\ell_N; k),$$

where  $c_{S_X}(\ell; k)$  denotes the number of composition of  $\ell$  with exactly  $k$  parts, each of which is in  $S_X$ . Accordingly, when  $\ell_1 = \cdots = \ell_N = \ell$  and all base sets are identical to some set  $S_X$ , then this becomes

$$a_S(\ell, \dots, \ell) = \sum_{k \geq 0} c_{S_X}(\ell; k)^N.$$

When, e.g.,  $S_X = \{1, \dots, M\}$ , for some  $M \geq 1$ , then the numbers  $c_{S_X}(\ell; k)$  are unimodal in  $\ell$  for fixed  $k$  (see [4, 5, 6]) and may be approximated by a normal curve as in [14].

5.5. *The case  $S = \{(s_1, \dots, s_N) \mid 0 \leq s_i \leq 1\} - \{\mathbf{0}_N\}$*

This is the classical case of alignments of  $N$  sequences considered in computational biology. An exact formula for  $a_S(\ell_1, \dots, \ell_N)$  is given by (see [32])

$$\sum_{k=\max\{\ell_1, \dots, \ell_N\}}^{\ell_1 + \dots + \ell_N} \sum_{j=0}^k (-1)^j \binom{k}{j} \prod_{j=1}^N \binom{k-j}{\ell_j}. \quad (2)$$

Eq. (2) can be derived via the inclusion/exclusion principle very similarly as above in Section 5.2.2. Another closed-form formula is given in a comment to integer sequence A126086, namely:

$$a_S(\ell_1, \dots, \ell_N) = \sum_{\mu \geq 0} \binom{\mu}{\ell_1} \cdots \binom{\mu}{\ell_N} \cdot \frac{1}{2^{\mu+1}}. \quad (3)$$

An approximate formula for  $a_S(\ell, \dots, \ell)$  has also been established (see [17, 28]):

$$a_S(\ell, \dots, \ell) \sim (2^{1/N} - 1)^{-N\ell} \frac{1}{(2^{1/N} - 1) 2^{(N^2-1)/2N} \sqrt{N(\pi\ell)^{N-1}}}.$$

### 5.6. The case $S = \mathbb{N}^N - \{\mathbf{0}_N\}$

In the case when no non-zero step from  $\mathbb{N}^N$  is discarded, a formula is given by (see [2]):

$$a_S(\ell_1, \dots, \ell_N) = \sum_{k \geq 0}^{\ell_1 + \dots + \ell_N} \sum_{i=0}^k (-1)^i \binom{k}{i} \prod_{j=1}^N \binom{\ell_j + k - i - 1}{\ell_j}.$$

It has been noted (see [10]) that  $a_{\mathbb{N}^N - \{\mathbf{0}_N\}}(\ell, \dots, \ell) = 2^{\ell-1} a_{\{(s_1, \dots, s_N) \mid 0 \leq s_i \leq 1\} - \{\mathbf{0}_N\}}(\ell, \dots, \ell)$ , which leads to the formula

$$a_{\mathbb{N}^N - \{\mathbf{0}_N\}}(\ell, \dots, \ell) = \sum_{\mu \geq 0} \binom{\mu}{\ell}^N 2^{\ell - \mu - 2}.$$

### 5.7. The case $S = \{(s_1, \dots, s_N) \mid 1 \leq s_i \leq 2\}$

As a closed-form formula for this case, we obtain as a specialization of our above results in Section 5.4:

$$a_S(\ell_1, \dots, \ell_N) = \sum_{k \geq 0} \prod_{i=1}^N \binom{\ell_i - k}{k}.$$

To derive an asymptotic formula for  $a_S(\ell, \dots, \ell)$ , we resort to the techniques for computing asymptotics of diagonal coefficients of multivariate generating functions (see [27, 28]). This leads us to the following theorem.

**Theorem 4** *Let  $\phi = \frac{\sqrt{5}-1}{2}$ . Moreover, let  $A = -\phi^{N-1}(1+\phi)^{N-1}(1+2\phi)$ . Define  $h = N \left( \frac{\phi}{1+3\phi+2\phi^2} \right)^{N-1}$  and  $b_0 = \frac{1}{-\phi A \sqrt{(2\pi)^{N-1} h}}$ . Then*

$$a_S(\ell, \dots, \ell) \sim \phi^{-\ell N} b_0 \ell^{(1-N)/2}.$$

*Proof.* Let  $\frac{I(\mathbf{z})}{J(\mathbf{z})} = \frac{1}{1 - \sum_{\mathbf{s} \in S} \mathbf{z}^{\mathbf{s}}}$  be the multivariate generating function for the number of  $S$ -alignments, with  $S$  as indicated. With notation as in [28], we call  $\text{CRIT}(\ell, \dots, \ell)$  the set of solutions  $\mathbf{x} \in \mathbb{R}^N$  satisfying  $J(\mathbf{x}) = 0$  and  $\ell x_i \frac{\partial J(\mathbf{x})}{\partial z_i} = \ell x_N \frac{\partial J(\mathbf{x})}{\partial z_N}$  (for all  $i < N$ ). Then,  $\text{CRIT}(\ell, \dots, \ell)$  is finite and there is exactly one contributing point  $\mathbf{c} = (\phi, \dots, \phi)$ , as defined in [28]. We find  $\phi$  by induction on  $N$ , starting from  $N = 1$ :  $1 - x - x^2 = 0$ ; in general, we consider the positive real root of  $1 - \sum_{i=0}^N \binom{N}{i} x^{N+i}$ . Finally, we apply Proposition 3.4 and Theorems 3.1-3.3 in [28] to derive the asymptotic.  $\square$

**Example 4** Table 5 compares the numbers  $a_S(\ell, \ell, \ell)$  for  $S_0 = \{(s_1, s_2, s_3) | 1 \leq s_i \leq 2\}$  and  $S_1 = \{(s_1, s_2, s_3) | 0 \leq s_i \leq 1\} - \{\mathbf{0}_3\}$ , respectively. We note that the latter numbers grow much more rapidly. In fact, under  $S = S_0$ ,  $a_S(10, 10, 10)$  is still quite moderate (68933), while under  $S = S_1$ , this number amounts to almost  $10^{16}$ .

$\ell$	$\{(s_1, s_2, s_3)   1 \leq s_i \leq 2\}$	$\{(s_1, s_2, s_3)   0 \leq s_i \leq 1\} - \{\mathbf{0}_3\}$
1	1	13
2	2	409
3	9	16081
4	29	699121
5	92	32193253
6	343	1538743249
7	1281	75494983297
8	4720	3776339263873
9	17899	191731486403293
10	68933	9850349744182729

Table 5: Comparing numbers for cases of Sections 5.5 and 5.7. Numbers are calculated via Theorem 1.

**Example 5** We let  $N = 3$ , and  $S = \{(1, 1, 1), (2, 1, 1), (1, 2, 1), (1, 1, 2), (2, 2, 1), (2, 1, 2), (1, 2, 2), (2, 2, 2)\}$ . Table 6 sketches exact and approximate values, computed from Theorem 4, of  $a_S(\ell, \ell, \ell)$  for  $\ell = 1, \dots, 20$ , and approximation errors.

## References

- [1] H. ANDRADE, I. AREA, J. J. NIETO, A. TORRES, The number of reduced alignments between two DNA sequences. *BMC Bioinformatics* **15** (2014), 94.  
<http://dx.doi.org/10.1186/1471-2105-15-94>
- [2] G. E. ANDREWS, The Theory of Partitions, II: Simon Newcom’s problem. *Utilitas Math.* **7** (1975), 33–54.
- [3] C. BANDERIER, S. SCHWER, Why Delannoy numbers? *Journal of Statistical Planning and Inference* **135** (2005) 1, 40 – 54.  
<http://www.sciencedirect.com/science/article/pii/S0378375805000534>

$\ell$	(I) $a_S(\ell, \ell, \ell) =$	(II) $a_S(\ell, \ell, \ell) \sim$	$\frac{ (I)-(II) }{(I)}$
1	1	1.6489	0.393
2	2	3.4924	0.427
3	9	9.8626	0.087
4	29	31.334	0.074
5	92	106.19	0.133
6	343	374.84	0.084
7	1281	1361.00	0.058
8	4720	5044.70	0.064
9	17899	18995.30	0.057
10	68933	72418.85	0.048
11	266364	278882.88	0.044
12	1037423	1082919.63	0.042
13	4072439	4234450.32	0.038
14	16065148	16656175.18	0.035
15	63658521	65852910.95	0.033
16	253356763	261522569.36	0.031
17	1012049086	1042661064.91	0.029
18	4055596343	4171406306.87	0.027
19	16299779331	16740341694.65	0.026
20	65683233938	67367564115.86	0.025

Table 6: Exact and approximate values of  $a_S(\ell, \ell, \ell)$  for  $S = \{(s_1, s_2, s_3) \mid 1 \leq s_i \leq 2\}$ . Exact numbers are calculated via Theorem 1.

- [4] H. BELBACHIR, Determining the mode for convolution powers of discrete uniform distribution. *Probability in the Engineering and Informational Sciences* **25** (2011) 4, 469–475.
- [5] H. BELBACHIR, F. BENCHERIF, L. SZALAY, Unimodality of certain sequences connected with binomial coefficients. *Journal of Integer Sequences [electronic only]* **10** (2007) 2, Article 07.2.3, 9 p., electronic only.
- [6] H. BELBACHIR, L. SZALAY, Unimodal rays in the ordinary and generalized Pascal triangles. *Journal of Integer Sequences [electronic only]* **11**

- (2008) 2, Article ID 08.2.4, 7 p., electronic only.
- [7] M. BÓNA, A. KNOPFMACHER, On the Probability that Certain Compositions Have the Same Number Of Parts. *Ann. Comb.* **14** (2010), 291–306.
  - [8] M. A. COVINGTON, Alignment of Multiple Languages for Historical Comparison. In: *Proceedings of the 36th Annual Meeting of the Association for Computational Linguistics and 17th International Conference on Computational Linguistics - Volume 1*. ACL '98, Association for Computational Linguistics, Stroudsburg, PA, USA, 1998, 275–279.  
<http://dx.doi.org/10.3115/980845.980890>
  - [9] M. A. COVINGTON, The Number of Distinct Alignments of Two Strings. *Journal of Quantitative Linguistics* **11** (2004) 3, 173–182.  
<http://dx.doi.org/10.1080/0929617042000314921>
  - [10] E. DUCHI, R. SULANKE, The  $2^{n-1}$  factor for multi-dimensional lattice paths with diagonal steps. *Séminaire Lotharingien de Combinatoire [electronic only]* **51** (2004), B51c, 16 p., electronic only.
  - [11] S. EGER, The Combinatorics of String Alignments: Reconsidering the Problem. *Journal of Quantitative Linguistics* **19** (2012) 1, 32–53.  
<http://dx.doi.org/10.1080/09296174.2011.638792>
  - [12] S. EGER, Restricted weighted integer compositions and extended binomial coefficients. *Journal of Integer Sequences [electronic only]* **16** (2013) 1, Article 13.1.3, 25 p., electronic only.
  - [13] S. EGER, Sequence alignment with arbitrary steps and further generalizations, with applications to alignments in linguistics. *Inf. Sci.* **237** (2013), 287–304.  
<http://dx.doi.org/10.1016/j.ins.2013.02.031>
  - [14] S. EGER, Stirling's approximation for central extended binomial coefficients. *The American Mathematical Monthly* **121** (2014) 4, 344–349.
  - [15] S. EGER, Multiple Many-to-Many Sequence Alignment for Combining String-Valued Variables: A G2P Experiment. In: *Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing of the Asian Federation of Natural Language Processing, ACL 2015, July 26-31, 2015, Beijing, China, Volume 1: Long Papers*. 2015, 909–919.  
<http://aclweb.org/anthology/P/P15/P15-1088.pdf>
  - [16] I. M. GESSEL, J. LI, Compositions and Fibonacci identities. *Journal of Integer Sequences [electronic only]* **16** (2013) 4, Article 13.4.5, 16 p., electronic only.

- [17] J. R. GRIGGS, P. HANLON, A. M. ODLYZKO, M. S. WATERMAN, On the number of alignments of  $k$  sequences. *Graphs and Combinatorics* **6** (1990) 2, 133–146.  
<http://dx.doi.org/10.1007/BF01787724>
- [18] S. HEUBACH, T. MANSOUR, Compositions of  $n$  with parts in a set. *Congressus Numerantium* **168** (2004), 253–266.
- [19] S. JIAMPOJAMARN, G. KONDRAK, T. SHERIF, Applying Many-to-Many Alignments and Hidden Markov Models to Letter-to-Phoneme Conversion. In: C. L. SIDNER, T. SCHULTZ, M. STONE, C. ZHAI (eds.), *HLT-NAACL*. The Association for Computational Linguistics, 2007, 372–379.  
<http://dblp.uni-trier.de/db/conf/naacl/naacl2007.html#JiampojamarnKS07>
- [20] C. KIMBERLING, Enumeration of Paths, Compositions of Integers, and Fibonacci Numbers. *Fibonacci Quarterly* **39** (2001) 5, 430–435.
- [21] C. KISELMAN, Asymptotic properties of the Delannoy numbers and similar arrays. Available at <http://web.iku.edu.tr/ias/documents/kiselmanpaper.pdf>.
- [22] C. KISELMAN, Functions on discrete sets holomorphic in the sense of Ferrand, or monodiffic functions of the second kind. *Science in China A: Mathematics* **51** (2008), 604–619.
- [23] V. I. LEVENSHTAIN, Binary Codes Capable of Correcting Deletions, Insertions and Reversals. *Soviet Physics Doklady* **10** (1966), 707.
- [24] M. E. MALANDRO, Integer compositions with part sizes not exceeding  $k$ . Arxiv preprint, <http://arxiv.org/pdf/1108.0337.pdf>.
- [25] E. MUNARINI, M. PONETI, S. RINALDI, Matrix compositions. *Journal of Integer Sequences* (2009).
- [26] B. J. OOMMEN, String Alignment with Substitution, Insertion, Deletion, Squashing, and Expansion Operations. *Inf. Sci. Inf. Comput. Sci.* **83** (1995) 1-2, 89–107.  
[http://dx.doi.org/10.1016/0020-0255\(94\)00110-W](http://dx.doi.org/10.1016/0020-0255(94)00110-W)
- [27] R. PEMANTLE, M. C. WILSON, Twenty Combinatorial Examples of Asymptotics Derived from Multivariate Generating Functions. *SIAM Review* **50** (2008) 2, 199–272.  
<http://dx.doi.org/10.1137/050643866>
- [28] A. RAICHEV, M. C. WILSON, A New Method for computing asymptotics of diagonal coefficients of multivariate generating functions. In: *2007 Conference on Analysis of Algorithms, AofA 07*. 2007, 439–449.

- [29] Ø. J. RØDSETH, J. A. SELLERS, Improving calculations of the number of distinct alignments of two strings. *Journal of Quantitative Linguistics* **13** (2006) 1, 45–55.  
<http://dx.doi.org/10.1080/09296170500500777>
- [30] C. SHAPCOTT, New bijections from  $n$ -color compositions. *Journal of Combinatorics* **4** (2013), 373–385.
- [31] N. J. A. SLOANE, The On-Line Encyclopedia of Integer Sequences.
- [32] J. B. SLOWINSKI, The Number of Multiple Alignments. *Molecular Phylogenetics and Evolution* **10** (1998) 2, 264 – 266.  
<http://www.sciencedirect.com/science/article/pii/S105579039890522X>
- [33] R. STANLEY, *Enumerate Combinatorics*. 1, 2 edition, Cambridge University Press, 2012.
- [34] A. TORRES, A. CABADA, J. J. NIETO, An Exact Formula for the Number of Alignments Between Two DNA Sequences. *DNA Sequence* **14** (2003), 427–430.